

# Mechanism for Aqueous Glycine Condensation

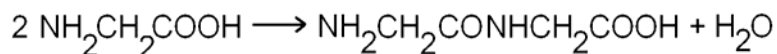
Robert Vergenz,<sup>\*§</sup> Eric V. Dornshuld,<sup>\*</sup> Ramy Mourad<sup>\*</sup> and Henry F. Schaefer III<sup>§</sup>

Sanibel Symposium, February, 2008, St. Simons Island, GA, USA

<sup>\*</sup> Department of Chemistry and Physics, University of North Florida  
Jacksonville, FL 32224-2645 USA

<sup>§</sup> Center for Computational Quantum Chemistry and Department of Chemistry  
University of Georgia, Athens, GA 30602-2525 USA

We investigate the mechanism for aqueous glycine condensation,



The MP2/6-31G\* model chemistry is used to calculate structures and energies of minima and maxima on a reaction coordinate diagram. Results for optimized reactant pair complex, two intermediates, and products are reported. The reactant pair complex had a C-N bond interaction distance of 2.8Å. The first intermediate has a glycyglycine backbone with multiple waters of hydration forming ring-like structures bridging the central carboxylic oxygen atoms with adjacent amine hydrogen atoms, with a C-N bond distance of 1.60Å. The second intermediate has a glycyglycine backbone with two hydroxyl groups on the carbon atom of the incipient peptide bond, and a C-N bond distance of 1.44Å. The product peptide bond distance is 1.37 Å.